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Subject: **Re-assessment of PMIC measurements for the determination of CTE of SA 508 steel**

This letter presents a summary of an assessment of measurement data for the determination of coefficient of thermal expansion (CTE) of SA 508 steel. The assessment shows that care is required when a regression curve is used to determine average CTE values since errors can be introduced by local lack-of-fit of the regression curve. A robust fit that faithfully represents the data trends allows valid average CTE values to be obtained from the fit.

Summary

An initial analysis of data collected by PMIC for the measurement of coefficient of thermal expansion (CTE) of SA508 was based on a polynomial fit to the raw data over the full temperature range of about 75 °F to about 1300 °F. Use of this fit to derive average CTE as a function of temperature resulted in values that were significantly lower than expectation up to a temperature of about 300 °F. Further scrutiny revealed several minor anomalies in the data and, most importantly, it was found that the raw data trend was not well represented by the polynomial fit in this temperature range. This difficulty can be addressed by the choice of a more representative curve fit. For this purpose, the LOWESS (locally weighted least squares regression) method offers a relatively straightforward and robust approach and avoids the need to find a suitable, global functional relationship. Applying such a weighted fit to the data collected by PMIC for this alloy in air, using a smoothing parameter of 0.1 (10%), was found to more faithfully represent the data trend up to 300 °F. Average CTE values determined from this curve fit compared well with the expected range. It is concluded, therefore, that this data set need not be rejected on the basis of the anomalies and that acceptable CTE results are obtained by ensuring that the curve fit faithfully follows important trends in the raw data and provides enough smoothing to reduce measurement noise.

Original and revised curve fits and CTE variation with temperature

Figure 1 shows details of the measured data up to a temperature of 300 °F and clearly shows the deviation of the polynomial fit from the measurements. This fit underestimates the slope at the lower temperatures and exaggerates the rate of change with increasing temperature. Figure 2 shows the same region of the data but with a LOWESS fit at a smoothing parameter of 10%. This fit clearly provides a truer representation of the data over this temperature range. The relative quality of the fits is further illustrated in Figure 3 which shows a plot of the residuals from both curve fits. The residuals to the polynomial fit show clear local deviations beyond the general, random measurement noise whereas the residuals to the LOWESS fit show only random elements. It is concluded from the *goodness* of the LOWESS fit that derived values of CTE will be reliable over the whole temperature range of the measurements.

Figure 4 presents a graph of the average CTE vs. temperature derived from both the original polynomial fit and from the LOWESS fit. Also shown in this figure is the average CTE taken from the 1998 ASME tables. The artificially low CTE produced by the polynomial fit for temperatures between 70 °F and 300 °F are clearly apparent. The CTE from the LOWESS fit is better behaved and agrees well with the ASME values.

Other data

The data for SA-508 collected in vacuum is subject to the same polynomial fitting problems as the data in air; however, this data contains features which appear to be other than random noise. These are particularly apparent at low temperatures and further consideration is required before attempting a different curve fit. However, at higher temperatures, CTE values from this data are in reasonable agreement with expectation with just the initial polynomial fit.

Sincerely,

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Reference for the LOWESS method of curve fitting: **Chambers, J. M., Cleveland, W. S., Kleiner, B., and Tukey, P. A. Graphical Methods for Data Analysis . Duxbury Press, Boston (1983)**.

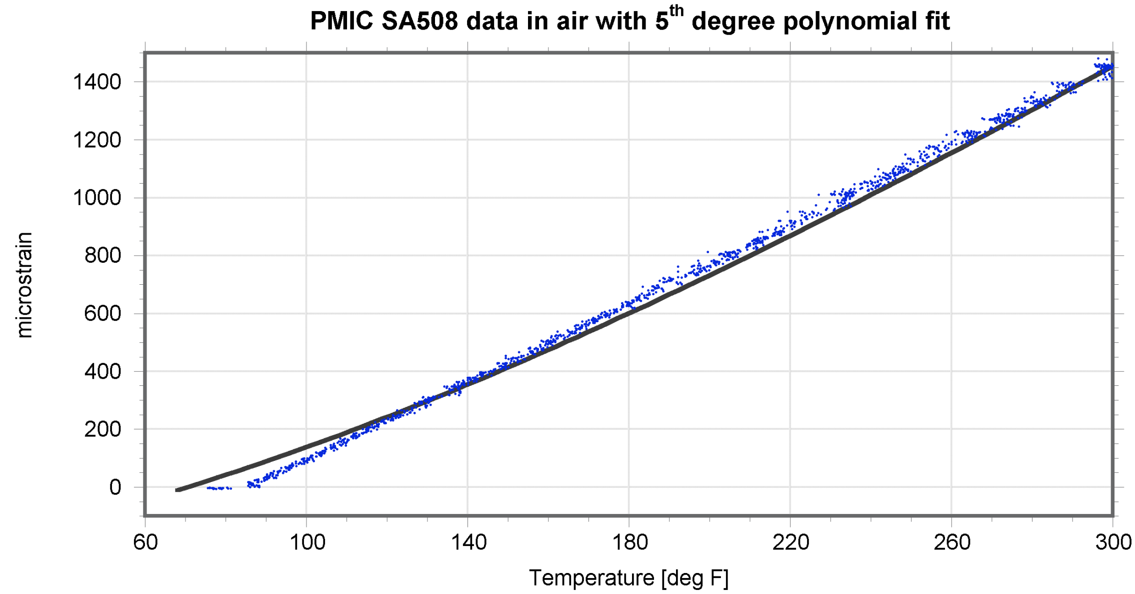

Figure 1 The low temperature part of the data is shown in detail in this plot together with the 5th degree polynomial fit. This curve fit clearly fails to represent the data well over this temperature range, even though the regression coefficient over the whole data range is very close to 1. The fit underestimates the initial slope and exaggerates the rate of change. These deviations can be seen in the residuals plotted in **Figure 3** and the corresponding effect on apparent average CTE is shown in **Figure 4**.

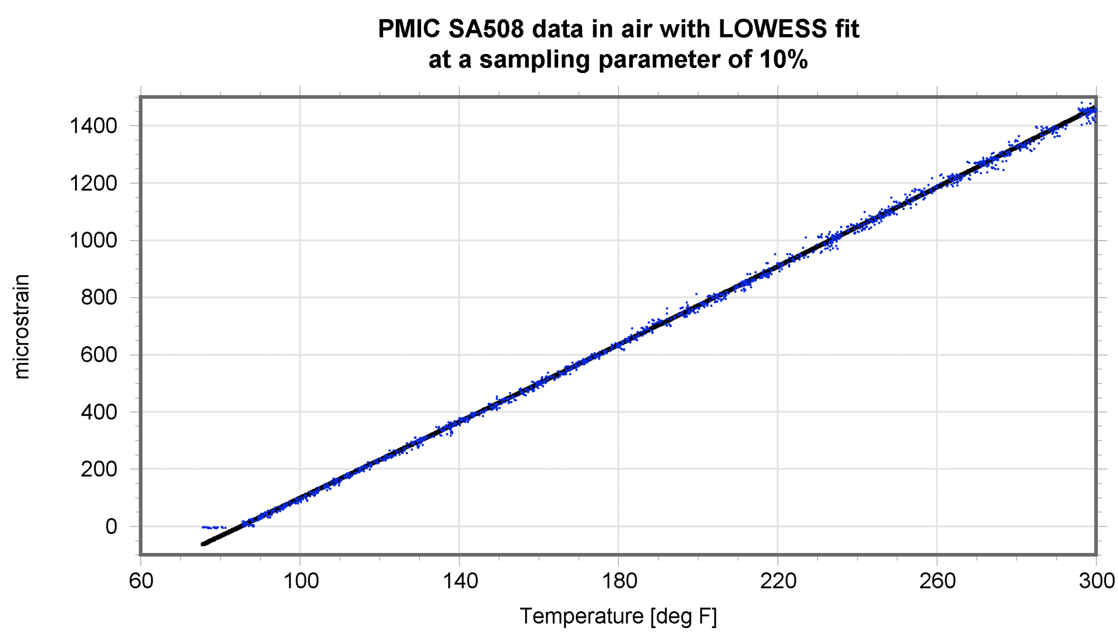

Figure 2 The low temperature part of the data is shown in detail in this plot together with the LOWESS fit. This curve fit faithfully represents the data well over this temperature range. The fit does not capture the initial horizontal portion of the curve, which is desirable since this is probably an experimental artifact rather than part of the true material response. The residuals plotted in **Figure 3** reflect the goodness of fit shown here and the corresponding apparent average CTE trend shown in **Figure 4** is close to expectation.

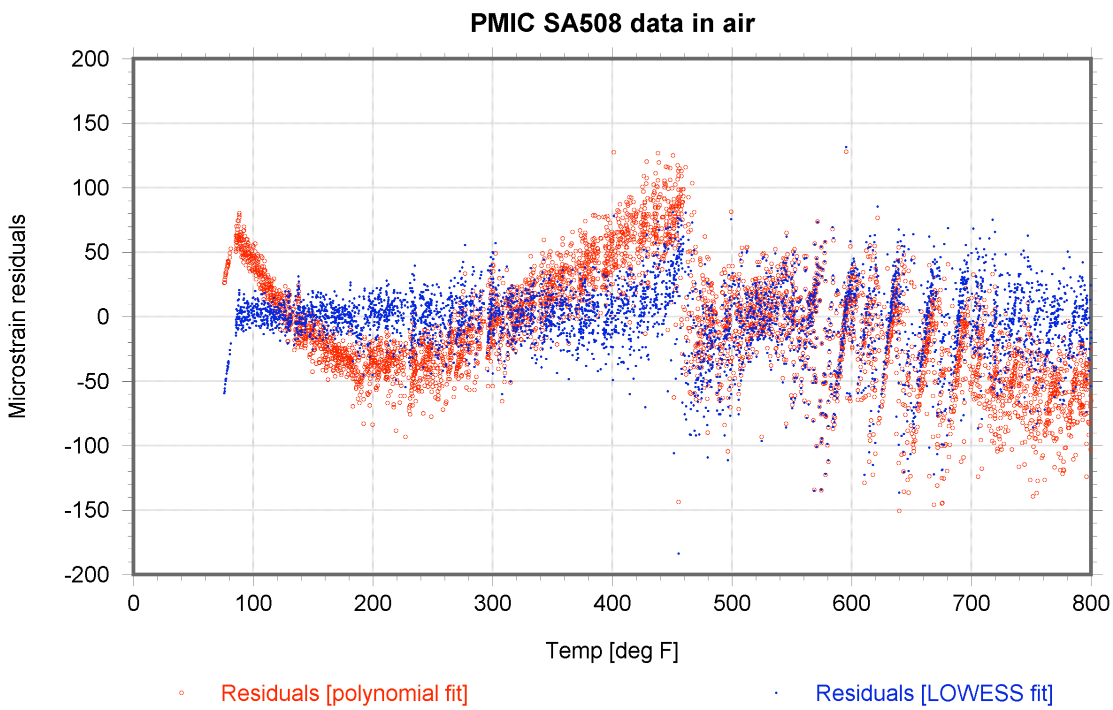

Figure 3 This figure shows the residuals of the microstrain measurements from two curve fits. It can be seen that the LOWESS residuals contain only random noise except for a minor perturbation at about 450 °F. The polynomial residuals, on the other hand deviate significantly from random noise behaviour. This leads to errors in determinations of average CTE at low temperatures.

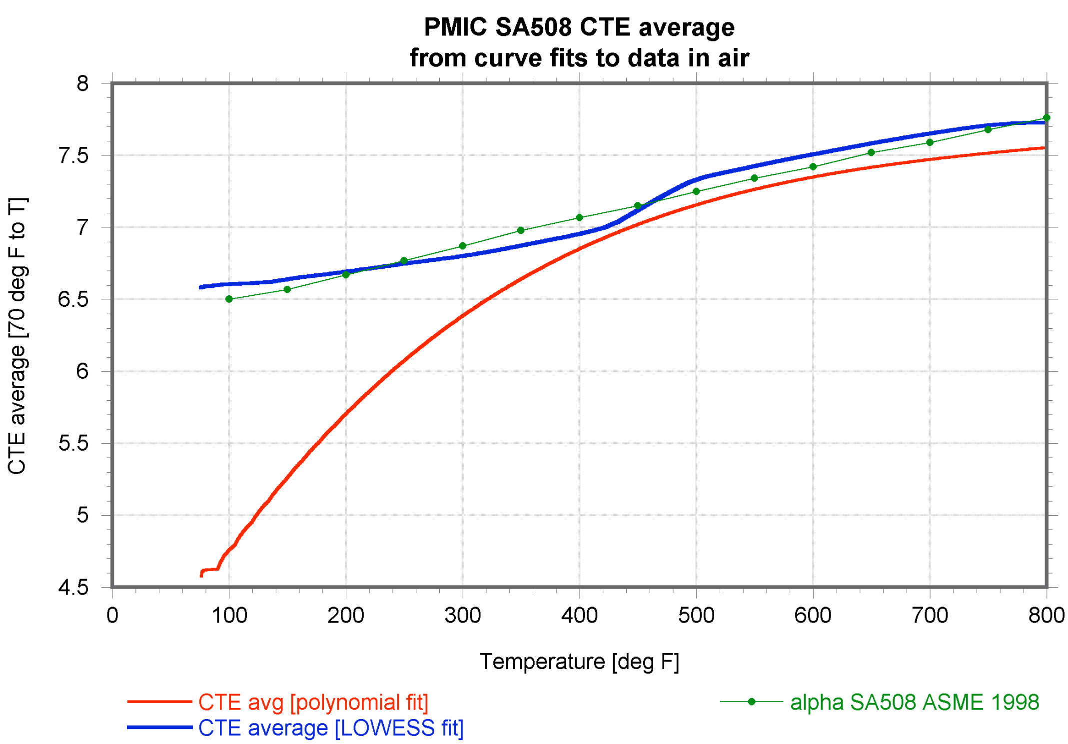

Figure 4 This plot shows the average CTE [70 °F to T] as calculated from the curve fits to the PMIC microstrain – temperature data collected in air. The ASME values tabulated for code year 1998 are shown for comparison. Calculated CTE values from the LOWESS fit agree well with the ASME values.